AB INITIO PREDICTIONS: CRITERIA FOR EVALUATION

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Measures implemented in the ACE package are described. In the evaluation of secondary structure predictions (1D) we discuss the Q index, segment overlap measure (SOV), and the statistics of segment discreteness (brakes/joints). For the 2D predictions we evaluate the contacts between segments of secondary structure and contacts between residues. In the case of 3D predictions RMS deviations in atomic positions and dihedral angles are calculated for all atoms and several subsets including secondary structure elements, core and surface residues, as well as side chains that are not reliable crystallographically. 1D and 2D characteristics are extracted from 3D predictions and evaluated as well.